Exercise series 4 22.10.2010

Linear Response, Kramers-Kronig relations, Lindhard function

Motivation Some basic properties of matter depend on its equilibrium state in quite an obvious manner. The density for instance is just the number of particles in a unit volume in equilibrium. Other important properties do not show up as expectation values in equilibrium, at least not in any obvious way. For example, the conductivity  $\hat{\sigma}$ , defined by  $\mathbf{j} = \hat{\sigma} \mathbf{E}$  is a basic property of matter, but it describes the system *response* in the form of current **j** to the the external electric field **E**. Such quantities are known as response functions. For weak external influences they are related to the correlations that exist in the system at equilibrium. This connection between the system response to weak perturbation and the correlation in equilibrium is established through the Kubo formula. In this set of exercises you are going to examine this connection and write down the general form of the conductivity for a noninteracting electron gas.



Fig. 1.3. Response functions are usually measurable experimentally.

Figure 1: Taken without permission from A. Tsvelik, Quantum Field Theory in Condensed Matter Physics, Cambridge University Press, Cambridge UK, 1995.

**Exercise 1: Kramers-Kronig relations (5 points)** The Kubo formula connects the response functions with the correlations in the equilibrium. Another view at this relation connects the response of the system to a change caused by regular external perturbation and the change in the system state due to fluctuations in the equilibrium. This view goes by the name of fluctuation-dissipation relations. One manifestation of such a relation are Kramers-Kronig relations. They connect the real and the imaginary part of an arbitrary response function. The real part of the response function describes the transmission of the external perturbing field. The imaginary part describes its dissipation. In this problem you are going to derive the Kramers-Kronig relations and discuss their significance. Also you will begin to feel at home in the complex plane. For an easy but insightful review of the most important aspects of the complex analysis, look at Byron and Fuller's text *Mathematics of Classical and Quantum physics*.

(a) Some response function is characterized by the susceptibility  $\chi(\mathbf{r}, t)$ . In a homogeneous system in equilibrium, the system's response  $R(\mathbf{r}, t)$  to the perturbation  $P(\mathbf{r}, t)$  is given by

$$R(\mathbf{r},t) = \int d\mathbf{r}' dt' \chi(\mathbf{r} - \mathbf{r}', t - t') P(\mathbf{r}', t').$$
(1)

For concreteness, we can think about R as the magnetization and P as the external magnetic field. The causality puts some constraints on the possible forms of the response function  $\chi$ . For example, it is possible to choose  $\chi$  in (1) so that the system response  $R(\mathbf{r}, t)$  depends on the perturbation at the position  $\mathbf{r}'$  and at time t' that are separated by a time-like interval. To avoid complications coming from the special relativity, we will in what follows consider the local response

$$R(\mathbf{r},t) = \int \mathrm{d}t' \chi(\mathbf{r},t-t') P(\mathbf{r},t').$$
(2)

When can we neglect the nonlocality of the response and work with (2) instead of the more general (1)?

(b) Taking the local response (2), what does the causality imply about the time dependence of susceptibility  $\chi(t)$  that connects the cause  $P(t_0 - t)$  and the effect at time  $t_0$ ?

(c) In linear response it is convenient to work with the Fourier transformed time dependence. The relation between the Fourier components of R and P takes the form

$$R(\omega) = \chi(\omega)P(\omega). \tag{3}$$

This simple form is a consequence of the fact that the Fourier transform of the convolution of two functions is the product of their Fourier transforms. The functions  $P(\omega)$ ,  $R(\omega)$ , and  $\chi(\omega)$ in (3) are Fourier transforms of the corresponding functions that appear in (2). Argue that the causality implies that the susceptibility is an analytic function of the complex frequency  $\omega$  in the upper half plane  $\text{Im}(\omega) > 0$ .

(d) Using the Cauchy theorem

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0} dz,$$
(4)

where the function f is analytic inside the contour C and continuous on C, and the fact that both  $P(\mathbf{r}, t)$  and  $R(\mathbf{r}, t)$  are real, show that the real and imaginary part of the susceptibility satisfy the Kramers-Kronig relations

$$\operatorname{Re}(\chi(\omega_0)) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\omega \operatorname{Im}(\chi(\omega))}{\omega^2 - \omega_0^2} \mathrm{d}\omega,$$
(5)

$$\operatorname{Im}(\chi(\omega_0)) = -\frac{\omega_0}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\operatorname{Re}(\chi(\omega))}{\omega^2 - \omega_0^2} \mathrm{d}\omega.$$
(6)

The symbol  $\mathcal{P}$  denotes the principal value of the integral and it is defined as

$$\mathcal{P}\int_{-\infty}^{\infty} f(x) \mathrm{d}x = \lim_{\epsilon \to 0} \left( \int_{-\infty}^{x_0 - \epsilon} f(x) \mathrm{d}x + \int_{x_0 + \epsilon}^{\infty} f(x) \mathrm{d}x \right),\tag{7}$$

where  $x_0$  is the point at which the function f has a singularity that makes it non-integrable.

(e) In the light of your calculation, explain the formula

$$\lim_{\epsilon \to 0^+} \frac{1}{x \pm i\epsilon} = \mathcal{P}\frac{1}{x} \mp i\pi\delta(x).$$
(8)

**Exercise 2: Lindhard function (5 points)** In this exercise we use the Kubo formula to calculate the susceptibility of the free electron gas. The relevant correlator in this case is between the particle densities

$$\chi^{R}(\mathbf{r} - \mathbf{r}', t - t') = -i\theta(t - t') \langle [\rho(\mathbf{r}, t), \rho(\mathbf{r}', t')] \rangle.$$
(9)

(a) When the perturbation is small (and this is the assumption behind Kubo formula) we are mostly interested in the linear response of the system. It is convenient to find the Fourier transform of the susceptibility

$$\chi^{R}(\mathbf{q}, t - t') = \int \mathrm{d}^{3}\mathbf{r}\chi^{R}(\mathbf{r} - \mathbf{r}', t - t')\mathrm{e}^{-i\mathbf{q}(\mathbf{r} - \mathbf{r}')}.$$
(10)

With the help of the Kubo formula, we can find the susceptibility in terms of real-space correlations  $\langle [\rho(\mathbf{r}, t), \rho(\mathbf{r}', t')] \rangle$ . Find this form of the susceptibility, and then express the real-space correlations in terms of the Fourier components of the density, defined by

$$\rho(\mathbf{r},t) = \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \rho(\mathbf{q},t).$$
(11)

(b) In the lectures you have seen that the particle density in momentum space is expressed in second quantized language by

$$\rho(\mathbf{q}) = \sum_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k}+\mathbf{q},\sigma}.$$
(12)

With the help of this definition and the canonical anticommutation relations, find the response function in the momentum space for free electrons. The result should be

$$\chi^{R}(\mathbf{q}, t - t') = -i\theta(t - t')\frac{1}{V}\sum_{\mathbf{k},\sigma} \left(n(\xi_{\mathbf{k}}) - n(\xi_{\mathbf{k}+\mathbf{q}})\right) e^{i(\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}})(t - t')},\tag{13}$$

where  $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$  is the excitation energy of the electron (or the electron energy measured with respect to the Fermi energy).

(c) Fourier transform the last expression once again, now with respect to time to obtain the Lindhard function

$$\chi^{R}(\mathbf{q},\omega) = \frac{1}{V} \sum_{\mathbf{k},\sigma} \frac{n(\xi_{\mathbf{k}}) - n(\xi_{\mathbf{k}+\mathbf{q}})}{\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}} + \omega + i\eta}.$$
(14)

In the last expression  $\eta > 0$  is a parameter that describes the adiabatic turning on and off of the interaction. It defines the precise position of the pole, which is crucial: For the *retarded* function we see that the poles for  $\omega$  are shifted slightly into the lower half-plane. The expression in the denominator is the dispersion relation for the excitations of the free electron gas. Discuss which excitation energies are possible for a fixed momentum **q** (draw a figure).